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# Two Canonical Representations for Regularized High Angular Resolution Diffusion Imaging

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**Abstract.** Two canonical representations for regularization of unit sphere functions encountered in the context of high angular resolution diffusion imaging (HARDI) are discussed. One of these is based on spherical harmonic decomposition, and its one-parameter extension via Tikhonov regularization. This case is well-established, and is mainly reviewed for the sake of completeness. The second one is new, and is based on a higher order diffusion tensor decomposition. A homogeneous representation of this type has been proposed in the literature, but we show that this is inconvenient for the purpose of regularization. We instead construct a heterogeneous representation that can be regarded as "canonical", to the extent that its behaviour under regularization mimics that of spherical harmonics.

**Key words:** Tikhonov regularization, higher order diffusion tensors, spherical harmonics, high angular resolution diffusion imaging (HARDI), diffusion tensor imaging (DTI), scale space.

## 1   Introduction

High angular resolution diffusion imaging (HARDI)—and, as a special case, diffusion tensor imaging (DTI)—has the potential to provide unprecedented insight into the microstructure of fibrous tissue such as muscle and brain white matter. It is to date the only in vivo technique for studying the microstructure of such tissues. Since tissue degeneration may occur as a precursor of certain diseases, it holds the promise to become an essential diagnostic tool. In addition it may further our insight in anatomy and brain connectivity, cf. Alexander et al. in the context of neurotherapeutic applications of brain DTI [1].

In order to model the a priori unconstrained number of point measurements in HARDI, one is naturally led to an infinite-dimensional Hilbert space framework. Apart from the obvious risk of overfitting, lack of control on the overwhelming number of degrees of freedom greatly complicates analysis and visualization.

Regularization provides a way to control data complexity and to ensure manifest robustness. We will review some finite-order Tikhonov regularization schemes from the literature, as well as a recently introduced infinite-order scheme [2–8]. It has appeared natural in all cases to employ a basis of spherical harmonics [9, 10], and this is indeed the typical procedure followed in practice. (The main reason for this review is to make the paper self-contained; the reader is referred to cited literature for details.)

However, an alternative but equally interesting decomposition has been put forward by Özarslan and Mareci [11]. Instead of spherical harmonics the authors propose to use *homogeneous* polynomials confined to the unit sphere, as a generalization of DTI. The "higher order diffusion tensors" constructed accordingly are in principle capable of modeling raw HARDI data to any prescribed accuracy. Although there is some implicit regularization in the act of truncating the polynomial expansion at some finite order, akin to the regularizing effect of fitting acquisition data to a second order DTI tensor, the intention is primarily to capture *raw* data to any desired level of detail. Indeed, the higher order diffusion tensor model of Özarslan and Mareci is best appreciated as a DTI generalization.

However, unlike with DTI, which by construction has only six independent degrees of freedom per point [12–14], there is no explicit regularization of a general HARDI signal. The question thus presents itself whether the tensor model of Özarslan and Mareci admits regularization in a "natural" way, similar to the case of the spherical harmonic description. The answer is no, in the sense that the employed basis functions are not eigenfunctions of standard regularization operators. This implies that there exists no "simple" way of adapting the raw data coefficients in their polynomial expansion so as to obtain a corresponding regularized expansion. We therefore modify their scheme by instead considering a *heterogeneous* polynomial on the sphere, and exploiting intrinsic redundancy so as to make each homogeneous term an eigenfunction under regularization. As a result, our alternative higher order diffusion tensor model reconciles the tensor rationale championed by Özarslan and Mareci with the regularization rationale, without sacrificing the niceties exhibited by the spherical harmonic description in this context. The "trick" is basically to extract from a homogeneous polynomial representation of order $N$, say, all those degrees of freedom that can be expressed in terms of spherical harmonics of lower orders, which can then be reformatted into lower order polynomial terms, ultimately producing an equivalent, heterogeneous polynomial. This will be operationalized in the next section.

For simplicity we will collectively refer to various related representations that employ functions on the unit sphere simply as "HARDI". These include Tuch's orientation distribution function (ODF) [15], the higher order diffusion tensor model and the diffusion orientation transform (DOT) by Özarslan et al. [11, 16], Q-Ball imaging [2], and the diffusion tensor distribution model by Jian et al. [17]. Considerations in this paper pertain to all such representations.

## 2   Theory

### 2.1   Notation

Let $S : \Omega \to \mathbb{R}$ denote a raw HARDI (or HARDI-related, v.s.) signal confined to the unit sphere $\Omega : \|x\| = 1$, $x \in \mathbb{R}^3$. $\Omega$ may be parameterized using two coordinates, $\xi^\mu$, $\mu = 1, 2$, say. The components of the Riemannian metric for the unit sphere $\Omega$ embedded in Euclidean 3-space $\mathbb{R}^3$ are then given by[1]

$$g_{\mu\nu} = \frac{\partial x^i}{\partial \xi^\mu} \eta_{ij} \frac{\partial x^j}{\partial \xi^\nu} \,, \tag{1}$$

in which $\eta_{ij}$ are the components of the Euclidean metric of the embedding space (in Cartesian coordinates $\eta_{ij} = 1$ iff $i = j$, otherwise zero). With $D_\mu$ we denote the covariant derivative with respect to $x^\mu$ induced by the metric $g_{\mu\nu}$. Recall that by construction we have $D_\rho g_{\mu\nu} = 0$, whence also $D_\mu g = 0$, in which we have used the shorthand notation $g = \det g_{\mu\nu}$. This "covariant constancy" of the metric tensor in fact defines the covariant derivative [18], and plays a key role in partial integration in covariant variational formulations of regularization.

The spherical geometry of the problem naturally suggests the use of spherical coordinates ($\xi^1 = \theta, \xi^2 = \phi$):

$$\Omega : (x^1, x^2, x^3) = (\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta) \,. \tag{2}$$

### 2.2   Regularization via Spherical Harmonic Decomposition

We now consider regularization of a raw HARDI signal $S$. To this end, consider the following functional, in which $S_T : \Omega \to \mathbb{R}$ is a Tikhonov regularization of $S : \Omega \to \mathbb{R}$, viz. such that

$$E(S_T) = \int_\Omega \left( S(\xi) - S_T(\xi) \right)^2 + \sum_{k \geq 1} t_k D_{\mu_1} \ldots D_{\mu_k} S_T(\xi) D^{\mu_1} \ldots D^{\mu_k} S_T(\xi) \, D\xi \tag{3}$$

is minimal. The subscript $T$ refers to a sequence of nonnegative regularization parameters, $T = \{t_k\}_{k \in \mathbb{N}}$, on which the solution depends. $D^\mu$ is shorthand for $g^{\mu\nu}(\xi) D_\nu$, and $D\xi = \sqrt{g(\xi)} \, d\xi^1 d\xi^2$, denotes the invariant measure on $\Omega$ (in spherical coordinates $D\xi = \sin\theta \, d\theta \, d\phi$). The parameters $t_k \in T$ need to be chosen so as to ensure convergence of the integral. An obvious choice is to set all but one of them nonzero. Examples of this are first and second order Tikhonov regularization as proposed by Hess et al. [4] ($t_1 = t \in \mathbb{R}^+$, remaining ones zero), and Descoteaux et al. [2, 3] ($t_2 = t \in \mathbb{R}^+$, remaining ones zero). The resulting Euler-Lagrange equations are finite-order PDEs, and are easily solved relative

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[1] Index summation applies to pairs of identical upper and lower indices.

to the basis of spherical harmonics, using conventional spherical coordinates, Eq. (2), by virtue of the property

$$\Delta_\Omega Y_\ell^m(\theta, \phi) = -\ell(\ell+1) Y_\ell^m(\theta, \phi) \,, \tag{4}$$

in which $\Delta_\Omega = D_\mu\, D^\mu$ is the Laplace-Beltrami operator on the unit sphere $\Omega$, and $Y_\ell^m$ denote the spherical harmonics[2]

$$Y_\ell^m(\theta, \phi) = \sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}}\, e^{im\phi}\, P_\ell^m(\cos\theta) \,, \tag{5}$$

with $P_\ell^m$ the associated Legendre polynomials:

$$P_\ell^m(z) = \frac{(-1)^m}{2^\ell \ell!} \left(1-z^2\right)^{\frac{m}{2}} \frac{d^{\ell+m}}{dz^{\ell+m}} \left(z^2-1\right)^\ell \quad \text{(with } -1 \le z \le 1\text{)}. \tag{6}$$

With the help of polar coordinates and spherical harmonics, setting

$$S(\theta, \phi) = \sum_{\ell,m}^* c_{\ell m}(0)\, Y_\ell^m(\theta, \phi) \,, \tag{7}$$

in which the asterisk indicates summation over the effective indices $\ell \in \mathbb{Z}_0^+$, $m \in \{-\ell, -\ell+1, \ldots, \ell-1, \ell\}$, and

$$c_{\ell m}(0) = \int_0^{2\pi} \int_0^\pi S(\theta, \phi)\, Y_\ell^{-m}(\theta, \phi)\, \sin\theta d\theta d\phi \,, \tag{8}$$

minimizers of Eq. (3) can generically be written as

$$S_T(\theta, \phi) = \sum_{\ell,m}^* c_{\ell m}(T)\, Y_\ell^m(\theta, \phi) \,. \tag{9}$$

In the first order Tikhonov regularization scheme by Hess et al. [4] we have, using a self-explanatory change of function prototype for the coefficients,

$$c_{\ell m}(t) = \frac{c_{\ell m}(0)}{1 + t\,\ell(\ell+1)} \,. \tag{10}$$

In the second order scheme by Descoteaux et al. [2, 3] we have

$$c_{\ell m}(t) = \frac{c_{\ell m}(0)}{1 + t\,\ell^2(\ell+1)^2} \,, \tag{11}$$

and so forth. Another scheme that leads to convergence of Eq. (3) is obtained by taking

$$t_k = \frac{t^k}{k!} \,, \tag{12}$$

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[2] Cf. functions.wolfram.com for further properties of $Y_\ell^m$ and $P_\ell^m$.

yielding the spherical scale space representation

$$c_{\ell m}(t) = e^{-t\ell(\ell+1)} \, c_{\ell m}(0) \,, \tag{13}$$

which is the analogue of the $e^{-t\|\omega\|^2}$-attenuation of frequencies of scalar images in the Euclidean plane under Gaussian blurring[3] [19]. This scheme is particularly interesting for its connection to an abelian semigroup, since one may write

$$S_t(\theta, \phi) = e^{t\Delta_\Omega} \, S(\theta, \phi) \,. \tag{14}$$

It reproduces the first order scheme by a Laplace transform over $t \in \mathbb{R}_0^+$, cf. Florack et al. [8].

We end this brief review with the remark that all one-parameter regularization schemes of the types discussed above are qualitatively similar, and identical in their asymptotics. Let us now turn to the tensor formalism.

## 2.3   Regularization via Higher Order Diffusion Tensor Decomposition

Instead of Eq. (7) we now consider a decomposition of raw HARDI data into "higher order diffusion tensors", recall Eq. (2),

$$S_N(x) = \sum_{k=0}^{N} \mathscr{D}^{i_1 \ldots i_k} x_{i_1} \ldots x_{i_k} \quad \text{with } N \in \mathbb{N} \cup \{0, \infty\} \text{ and } S_\infty(x) \equiv S(x). \tag{15}$$

It should be realized that the collection of polynomials on the sphere,

$$\mathscr{B} = \bigcup_{k \in \mathbb{N} \cup \{0\}} \mathscr{B}_k \quad \text{with} \quad \mathscr{B}_k = \{x_{i_1} \ldots x_{i_k} \mid k \in \mathbb{N} \cup \{0\} \text{ fixed}\} \,, \tag{16}$$

is complete, but redundant. In fact, any order monomial of fixed parity can be obtained from a given higher order one of the same parity via contractions. There is no way to remove such redundancies from the *full* expansion, i.e. when $N = \infty$ in Eq. (15). However, if, following Özarslan and Mareci [11], one considers only the *approximation* corresponding to *finite* $N$, then mutual dependencies can be removed by setting all coefficients equal to zero except $\mathscr{D}^{i_1 \cdots i_N}$. The resulting homogeneous polynomial can then be fitted to the raw HARDI data as described by Özarslan and Mareci [11]. One then ends up with a representation of the form

$$S_N^{\ddot{\text{O}}.\text{M.}}(x) = D^{i_1 \ldots i_N} x_{i_1} \ldots x_{i_k} \quad \text{with } N \in \mathbb{N} \cup \{0\}, \tag{17}$$

as a generalization of the rank-2 DTI tensor. (By symmetry of the HARDI profile only even $N$ are relevant.) By construction, this polynomial representation is equivalent to the spherical harmonic decomposition, Eqs. (7–8), if the latter is constrained to include terms of orders $\ell \leq N$ only.

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[3] Koenderink's argument generalizes to Riemannian spaces without major difficulties.

Following the same rationale as in the context of a spherical harmonic decomposition, we would like to regularize the data representations of Eq. (15). That is, we seek corresponding regularized representations of the form[4]

$$S_N(x,t) = \sum_{k=0}^{N} \mathscr{D}^{i_1 \dots i_k}(t)\, x_{i_1} \dots x_{i_k} \quad \text{with } N \in \mathbb{N} \cup \{0, \infty\} \text{ and } S_\infty(x,t) \equiv S(x,t).$$

(18)

Of course, Eq. (17) *in principle* admits regularization in formally the same way:

$$S_N^{\ddot{\mathrm{O}}.\mathrm{M}.}(x,t) = D^{i_1 \dots i_N}(t)\, x_{i_1} \dots x_{i_k} \quad \text{with } N \in \mathbb{N} \cup \{0\},$$

(19)

which is just the tensorial counterpart of Eq. (9) (for the one-parameter case, and inclusion of terms $\ell \leq N$ only). However, whereas the spherical harmonics of fixed $\ell$ are eigenfunctions of the Laplace-Beltrami operator $\Delta_\Omega$, recall Eq. (4), this is *not* the case for any of the monomials in $\mathscr{B}_k$, Eq. (16). Consequently it is a nontrivial task to establish the coefficients $D^{i_1 \dots i_N}(t)$ as a function of $t$ in Eq. (19). Another drawback of the tensor representation in the form of Eq. (17) is that the coefficients depend on the truncation order $N$. Thus as soon as one alters $N$, *all* data information (as far as captured by the available degrees of freedom) will have to migrate to new tensor coefficients of corresponding rank.

In the formulation of our *Ansatz*, Eq. (15), we anticipate that only *residual* information is encoded in the higher order part of the heterogeneous polynomial, i.e. additional structure that cannot be revealed by a lower order polynomial. In fact we will construct the coefficients $\mathscr{D}^{i_1 \dots i_k}$ such that (i) they do not depend on $N$, and (ii) they transform upon regularization in a way quite similar to the coefficients $c_{\ell m}(t)$ in Eqs. (10), (11), or (13), depending on one's preferred choice of regularization paradigm. We are now in a position to formulate our main results. Detailed derivations and proofs can be found elsewhere [7].

We construct the coefficients according to the following algorithm.

**Algorithm 1** *Suppose we are in possession of $\mathscr{D}^{i_1 \dots i_k}$ for all $k = 0, \dots, N-1$, then minimization of the function*

$$E_N(\mathscr{D}^{j_1 \dots j_N}) = \int_\Omega \left( S(x) - \sum_{k=0}^{N} \mathscr{D}^{i_1 \dots i_k} x_{i_1} \dots x_{i_k} \right)^2 d\Omega,$$

*yields the following linear systems:*

$$\Gamma_{i_1 \dots i_N j_1 \dots j_N} \mathscr{D}^{j_1 \dots j_N} = \int_\Omega S(x)\, x_{i_1} \dots x_{i_N}\, d\Omega - \sum_{k=0}^{N-1} \Gamma_{i_1 \dots i_N j_1 \dots j_k} \mathscr{D}^{j_1 \dots j_k},$$

*with symmetric covariant tensor coefficients* $\Gamma_{i_1 \dots i_k} = \int_\Omega x_{i_1} \dots x_{i_k}\, d\Omega.$

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[4] We henceforth restrict our attention to the scheme of Eqs. (12–13), but the other one-parameter schemes discussed can be handled in a similar fashion.

The appearance of the second inhomogeneous term on the r.h.s. of the linear systems, absent in the scheme proposed by Özarslan and Mareci, reflects the fact that in our scheme higher order coefficients encode residual information only. The last integral is the tensorial counterpart of a well-known closed-form multi-index representation, cf. Folland [20] and Johnston [21], viz.:

$$\int_\Omega x_1^{\alpha_1} \ldots x_n^{\alpha_n}\, d\Omega = \frac{2}{\Gamma(\frac{1}{2}|\alpha| + \frac{n}{2})} \prod_{i=1}^{n} \Gamma(\tfrac{1}{2}\alpha_i + \tfrac{1}{2}), \qquad (20)$$

if all $\alpha_j$ are even (otherwise the integral vanishes). Here $|\alpha| = \alpha_1 + \ldots + \alpha_n$ denotes the norm of the multi-index, and

$$\Gamma(t) = \int_0^\infty s^{t-1}\, e^{-s}\, ds = 2 \int_0^\infty r^{2t-1}\, e^{-r^2}\, dr \qquad (21)$$

is the gamma function. Recall $\Gamma(\ell) = (\ell-1)!$ and $\Gamma(\ell+\frac{1}{2}) = (\ell-\frac{1}{2}) \ldots \frac{1}{2}\sqrt{\pi} = (2\ell)!\sqrt{\pi}/(4^\ell\, \ell!)$ for $\ell \in \mathbb{N} \cup \{0\}$. A translation from multi-index to tensor-index notation provides us with the closed-form of $\Gamma_{i_1 \ldots i_k}$:

**Result 1** *Cf. Algorithm 1 and Eqs. (20–21). In $n$ dimensions $\Gamma_{i_1 \ldots i_{2k+1}} = 0$, and*

$$\Gamma_{i_1 \ldots i_{2k}} = \frac{2\, \Gamma(k+\frac{1}{2})\Gamma(\frac{1}{2})^{n-1}}{\Gamma(k+\frac{n}{2})}\, \eta_{(i_1 i_2} \ldots \eta_{i_{2k-1} i_{2k})}\,.$$

*Parentheses denote complete symmetrization of indices. For $n = 3$ we obtain*

$$\Gamma_{i_1 \ldots i_{2k}} = \frac{2\pi}{k+\frac{1}{2}}\, \eta_{(i_1 i_2} \ldots \eta_{i_{2k-1} i_{2k})}\,.$$

Some examples ($n = 3$):

$$\Gamma = 4\pi\,, \quad \Gamma_{ij} = \frac{4\pi}{3}\, \eta_{ij}\,, \quad \Gamma_{ijk\ell} = \frac{4\pi}{15}\, (\eta_{ij}\, \eta_{k\ell} + \eta_{ik}\, \eta_{j\ell} + \eta_{i\ell}\, \eta_{jk})\,. \qquad (22)$$

It is straightforward to sequentially solve the linear systems in Algorithm 1. It follows that the scalar $\mathscr{D}$ is just the average value over the unit sphere:

$$\mathscr{D} = \frac{\int_\Omega S(x)\, d\Omega}{\int_\Omega d\Omega}\,. \qquad (23)$$

The constant vector $\mathscr{D}^i$ vanishes identically, as it should. For the rank-2 tensor coefficients we find the *traceless* matrix

$$\mathscr{D}_{ij} = \frac{15 \int_\Omega S(x)\, x_i\, x_j\, d\Omega - 5 \int_\Omega S(x)\, d\Omega\, \eta_{ij}}{2 \int_\Omega d\Omega}\,, \qquad (24)$$

and so forth. If, instead, we fit a homogeneous second order polynomial to the data (by formally omitting the second term on the r.h.s. of the linear systems

in Algorithm 1), as proposed by Özarslan and Mareci, we obtain the following rank-2 tensor coefficients:

$$D_{ij}^{\text{Ö.M.}} = \frac{15 \int_\Omega S(x) \, x_i \, x_j \, d\Omega - 3 \int_\Omega S(x) \, dx \, \eta_{ij}}{2 \int_\Omega d\Omega} \,, \qquad (25)$$

which is clearly different. However, Özarslan and Mareci's homogeneous expansion should be compared to our heterogeneous expansion. Indeed, if we compare the respective second order expansions in this way we observe that $S_2^{\text{Ö.M.}}(x) = S_2(x)$. The difference in coefficients, in this example, is explained by the contribution already contained in the lowest order term of our polynomial, which in Özarslan and Mareci's scheme has migrated to the second order tensor. In fact equality holds for any order $N$:

**Theorem 1** *Recall Eqs. (15) and (17). We have $S_N^{\text{Ö.M.}}(x) = S_N(x)$.*

The following theorem shows in which precise sense our new expansion can be called "canonical".

**Theorem 2** *If $\Delta_\Omega$ denotes the Laplace-Beltrami operator on the unit sphere, then for any $N \in \mathbb{N} \cup \{0, \infty\}$,*

$$S_N(x,t) \equiv e^{t\Delta_\Omega} \, S_N(x) = \sum_{k=0}^{N} \mathscr{D}^{i_1 \dots i_k}(t) \, x_{i_1} \dots x_{i_k} \,,$$

*with $\mathscr{D}^{i_1 \dots i_k}(t) = e^{-k(k+1)t} \, \mathscr{D}^{i_1 \dots i_k}$.*

The proof of Theorems 1–2 is presented elsewhere [7].

It seems somewhat miraculous that the $t$-scaling behaviour of the coefficients in Theorem 2 is identical to that in the spherical harmonic decomposition, Eq. (13). This is quite nontrivial, since the monomials $x_{i_1} \dots x_{i_k}$ are themselves not eigenfunctions of the Laplace-Beltrami operator. In fact, what happened is that, by considering the *specific* linear combinations $\mathscr{D}^{i_1 \dots i_k}(t) \, x_{i_1} \dots x_{i_k}$ according to the recipe of Algorithm 1, we have effectively disposed of the degrees of freedom in the monomials $x_{i_1} \dots x_{i_k}$ that live in eigenspaces spanned by the spherical harmonics $Y_\ell^m$ of orders $\ell < k$. The span of the resulting homogeneous polynomials coincides with the degenerate eigenspace of the $k$-th order spherical harmonics, span $\{Y_k^m \,|\, m \in \{-k, -k+1, \dots, k-1, k\} \,,\ k \in \mathbb{N} \cup \{0\}$ fixed$\}$.

Heuristically, the significance of Theorem 2 is that it segregates degrees of freedom in the polynomial expansion in such a way that we may interpret each homogeneous higher order term as an incremental refinement of detail relative to that of the lower order expansion. The linear combinations $\mathscr{D}^{i_1 \dots i_k} \, x_{i_1} \dots x_{i_k}$, unlike the monomials $x_{i_1} \dots x_{i_k}$ themselves, apparently constitute *self-similar*

*polynomials on the sphere* under the act of blurring by the regularization operator $\exp(t\Delta_\Omega)$, recall Eq. (14), or any of the other bounded one-parameter regularization operators previously reviewed, which are all of the form $f(t\Delta_\Omega)$ for suitably defined analytical function $f$. The parameter $t$ determines the angular resolution of the regularized data.

As a final observation we note that the classical rank-2 DTI representation, defined via the Stejskal-Tanner formula [11, 22]:

$$\Sigma(x) = \Sigma_0 \exp\left(-bS(x)\right) , \tag{26}$$

arises not merely as an approximation under the assumption that the diffusion attenuation can be written as

$$S(x) \approx S_{\mathrm{DTI}}(x) = D_{\mathrm{DTI}}^{ij} x_i x_j , \tag{27}$$

but, according to Theorem 2, expresses the *exact* asymptotic behaviour of $S(x,t)$ as $t \to \infty$:

$$\underbrace{\left(\mathscr{D}\,\eta^{ij} + e^{-6t}\,\mathscr{D}^{ij}\right) x_i\, x_j}_{S_{\mathrm{DTI}}(x,t)\,=\,D_{\mathrm{DTI}}^{ij}(t)\, x_i\, x_j} + \mathcal{O}(e^{-20t}) \quad (t \to \infty) . \tag{28}$$

This example shows that the higher order tensors constructed by Özarslan and Mareci in general, and the classical DTI tensor in particular, are not self-similar, but have a multimodal (respectively bimodal) resolution dependence, i.e. they contain multiple self-similar terms with different scaling behaviour under regularization. The actual limit of vanishing resolution is of course given by a complete averaging over the sphere, recall Eq. (23), noting that $\eta^{ij} x_i x_j = 1$ on $\Omega$:

$$\lim_{t\to\infty} S(x,t) = \lim_{t\to\infty} S_{\mathrm{DTI}}(x,t) = \mathscr{D} . \tag{29}$$

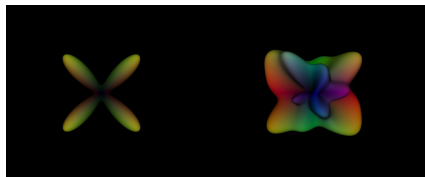See Figs. 1–2 for an illustration of Theorem 2 for $N = 8$ on a synthetic image.



**Fig. 1.** Left: Synthetic noise-free profile induced by two crossing fibers at right angle. Right: Same, but with Rician noise.
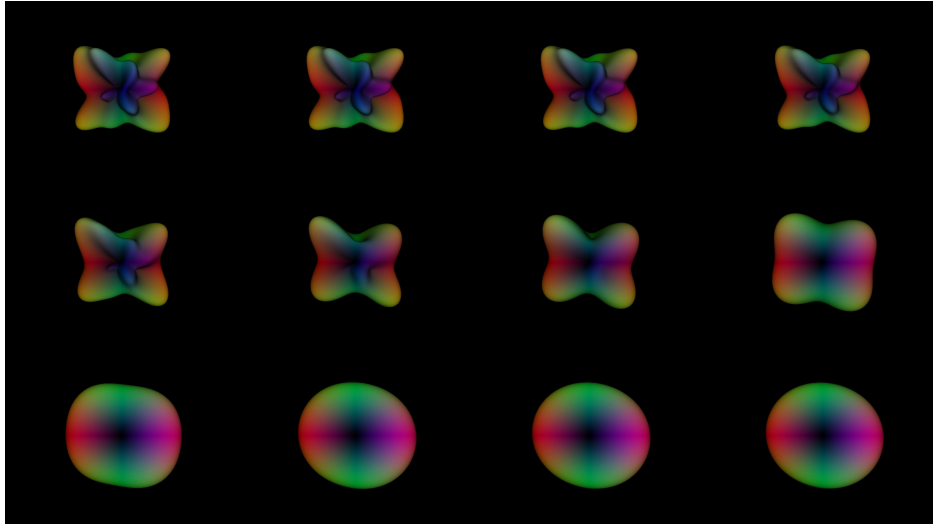
**Fig. 2.** Regularized profiles produced from the right image in Fig. 1 using Theorem 2 for $N = 8$. The regularization parameter $t$ increases exponentially from top left to bottom right over the range 0.007–1.0. For low $t$-values spurious peaks prevent correct detection of underlying fiber orientations. Peaks are gradually removed as $t$ increases. In the range $t \in [0.05, 0.15]$ we find two nearly correct peak locations intersecting at a stable angle of $82.5° \pm 0.8°$. For larger $t$ overregularization sets in as we enter the classical DTI regime, which is incapable of unconfounding crossing fibers.

## 3   Summary and Conclusion

We have considered two alternative representations for scalar functions on the sphere in the context of high angular resolution diffusion imaging (HARDI). One employs spherical harmonics, the second "higher order diffusion tensors".

The spherical harmonic representation is ideally suited for the application of various Tikhonov regularization schemes, associated with operators of the form $f(t\Delta_\Omega)$, in which $\Delta_\Omega$ is the Laplace-Beltrami operator on the sphere $\Omega$, and $f$ a suitably defined analytical function. This is a result of the fact that the spherical harmonics have a natural arrangement into orthogonal subsets of degenerate eigenfunctions of this operator, such that the closure of the direct sum of these subsets makes up $L_2(\Omega)$. This representation thus provides a natural ("canonical") framework for regularization.

If one wishes to employ a tensorial representation (or polynomials on the unit sphere), regularization becomes in general a highly nontrivial matter if one declines from an explicit projection onto the spherical harmonic basis. We have argued that the homogeneous tensorial representation proposed in their seminal paper by Özarslan and Mareci [11] is inconvenient in this respect. We have

operationally constructed an alternative, heterogeneous tensorial representation, which does mimic the "canonical" behaviour of the spherical harmonics.

Although all representations—spherical harmonics, higher order diffusion tensors by Özarslan and Mareci, and our newly constructed ones—are equivalent, there may be good reasons for preferring or excluding a particular one, as we have demonstrated in the context of regularization. A case where tensors may be preferred over spherical harmonics is in generalizing the differential geometric rationale for tractography and connectivity analysis via geodesics and geodesic congruences (Hamilton-Jacobi framework). For instance, it is most straightforward to construct a Finsler metric using a higher order diffusion tensor description, as a generalization of the DTI induced Riemannian metric, cf. Melonakos et al. [23].

In any case, regularization is an important procedure in HARDI, and so it is quite convenient to be able to carry it out irrespective of one's preferred paradigm. It remains an open question how to combine codomain regularization, as proposed here, with regularization in the spatial domain, cf. [24] in the context of DTI.

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